WHAT IS CLAIMED IS:

1.   A method, comprising:

defining an experimental space of a catalyzed chemical reaction to represent at least three factor interactions,

5   effecting a combinatorial high throughput screening (CHTS) method on the catalyzed chemical experimental space to produce results; and

analyzing the results according to matrix algebra to select a best case set of factor levels from the catalyzed experimental space.

2.   The method of claim 1, wherein the experimental space is

10   defined to represent all interactions of factors of the reaction.

3.   The method of claim 1, wherein the experimental space is defined according to a full factorial design.

4.   The method of claim 1, wherein the results from the matrix algebra analysis are represented according to a general linear model.

15   5.   The method of claim 1, wherein the experimental space is defined according to a full factorial design that represents at least 6 orders of interaction of factors of the reaction.

6.   The method of claim 1, wherein the experimental space is defined according to a full factorial design that represents at least 9 orders of

20   interaction of factors of the reaction.

7.   The method of claim 1, wherein the experimental space is defined according to a full factorial design that represents all orders of interaction of factors of the reaction.

8.   The method of claim 1, wherein the analyzing step comprises:

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(A) representing the results as an n x 1 matrix y where n = a number of factor level combinations in the experiment;

(B) representing extents of the factor level combinations in an n x n matrix X;

(C) solving n simultaneous equations represented by the matrices according to matrix algebra to form a results matrix β; and

(D) examining the results matrix β to identify effects outside a standard deviation.

9.   The method of claim 8, wherein (B) comprises coding extents of the factor level combinations as a +1 or −1 and representing the coded extents as the n x 1 matrix y.

10.   The method of claim 8, wherein (C) comprises:

(i) transposing matrix X to form matrix X';

(ii) postmultiplying X' by X to generate a matrix; and

(iii) postmultiplying the generated matrix by y to form the results matrix β.

11.   The method of claim 8, wherein (D) comprises:

(i) representing the results matrix β as a normal probability plot;

(ii) defining a standard deviation for results of the plot; and

(iii) identifying positive interactions outside of the standard deviation.

12.   The method of claim 11, wherein the standard deviation represents a probability that a result deviation from the standard is random and that a positive interaction can be identified outside of the deviation.

13.   The method of claim 12, wherein the probability is established at 95 percent or better.

14.   The method of claim 12, wherein the probability is established at 99.7 percent or better.

15.   The method of claim 11, wherein the positive interactions are results that represent a best set of factor levels from the experimental space.

16.   The method of claim 15, wherein the best set of factor levels defines leads for a commercial process.

17.   The method of claim 15, wherein the best set of factor levels defines a space for further investigation by reiteration of a CHTS method.

18.   The method of claim 1, wherein the matrix algebra analysis comprises representing the results according to the following model equation (I)

$$y = X\beta + e \qquad (I)$$

where X is a matrix of factor and interaction levels in the experiment, y is a matrix of experimental results, β is effects and e is an error term of variance σ^2 from a normal distribution.

19.   The method of claim 18, wherein the matrix algebra analysis comprises assembling results as an n x 1 vector y, assembling factor level values into an n x k+1 matrix X, representing extents of the results and factor level values as +1's and −1's accordingly and solving for effects parameters β according to the relationship:

$$\beta = (X'X)^{-1}X'y \qquad (II)$$

where superscript ' is a transpose of a matrix and superscript $^{-1}$ identifies an inverse function of a matrix.

.20. The method of claim 19, comprising examining the solved effects parameters β to identify effects outside a standard deviation.

21. The method of claim 20, further comprising reiterating the CHTS method wherein an experimental space for the CHTS method is selected according to the identified effects.

22. The method of claim 1, further comprising applying a statistical analysis to the results to identify interactions that represent a best set of factor levels from the experimental space.

23. The method of claim 1, wherein the CHTS comprises effecting parallel chemical reactions of an array of reactants defined as the experimental space.

24. The method of claim 1, wherein the CHTS comprises effecting parallel chemical reactions on a micro scale on reactants defined as the experimental space.

25. The method of claim 1, wherein the CHTS comprises an iteration of steps of simultaneously reacting a multiplicity of tagged reactants and identifying a multiplicity of tagged products of the reaction and evaluating the identified products after completion of a single or repeated iteration.

26. The method of claim 1, wherein the experimental space factors comprise reactants, catalysts and conditions and the CHTS comprises

(A) (a) reacting a reactant selected from the experimental space under a selected set of catalysts or reaction conditions; and (b) evaluating a set of results of the reacting step; and

(B) reiterating step (A) wherein a selected experimental space selected for a step (a) is chosen as a result of an evaluating step (b) of a preceding iteration of step (A).

27. The method of claim 26, wherein the evaluating step (b) comprises identifying relationships between factor levels of the candidate chemical reaction space; and determining the chemical experimental space according to a full factorial design for the next iteration.

28. The method of claim 26, comprising reiterating (A) until a best set of factor levels of the chemical experimental space is selected.

29. The method of claim 1, wherein the chemical space includes a catalyst system comprising a Group VIII B metal.

30. The method of claim 1, wherein the chemical space includes a catalyst system comprising palladium.

31. The method of claim 1, wherein the chemical space includes a catalyst system comprising a halide composition.

32. The method of claim 1, wherein the chemical space includes an inorganic co-catalyst.

33. The method of claim 1, wherein the chemical space includes a catalyst system includes a combination of inorganic co-catalysts.

34. The method of claim 1, wherein the defined space comprises a reactant or catalyst at least partially embodied in a liquid and effecting the CHTS method comprises contacting the reactant or catalyst with an additional reactant at least partially embodied in a gas, wherein the liquid forms a film having a thickness sufficient to allow a reaction rate that is essentially independent of a mass transfer rate of additional reactant into the liquid to synthesize products that comprise the results.

35.   A method of conducting an experiment, comprising steps of:

(A) conducting a CHTS experiment on a complex experimental space comprising qualitative and quantitative factors to produce first data results;

(B) analyzing the first data results according to matrix algebra;

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(C) defining a standard deviation of the analyzed results;

(D) selecting data results that positively exceed the standard deviation,

(E) defining a next experimental space according to the selected data results; and

(F) reiterating steps (A) through (E) on the next experimental space

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until data results selected in step (D) represent satisfactory leads.

36.   A system for investigating a catalyzed experimental space, comprising;

a reactor for effecting a CHTS method on the catalyzed chemical experimental space to produce results; and

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a programmed controller that analyzes the results according to matrix algebra to select a best case set of factor levels from the catalyzed experimental space.

37.   The system of claim 36, comprising a programmed controller that analyzes the results according to matrix algebra and represents the results of the analysis according to a substantially linear model.

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38.   The system of claim 36, comprising a programmed controller to define the catalyzed chemical experimental space to represent at least three factor interactions.

39.   The system of claim 36, wherein the controller is a computer, processor or microprocessor.

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40.   The system of claim 36, further comprising a dispensing assembly to charge factor levels of reactants or catalysts representing the catalyzed chemical experimental space to wells of an array plate for charging to the reactor.

41.   The system of claim 39, comprising a programmed controller to define the catalyzed chemical experimental space and to control the assembly to charge factor levels of reactants or catalysts according to the controller defined space.

42.   The system of claim 36, further comprising a detector to detect results of the CHTS method effected in the reactor.